

# wCorr Arguments

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This vignette explores two Boolean switches in the wCorr package. First, the `ML` switch allows for either a non-MLE (but consistent) estimate of the nuisance parameters that define the binning process to be used (`ML=FALSE`) or for the nuisance parameters to be estimated using the MLE (`ML=TRUE`). Second the `fast` argument gives the option to use a pure R implementation (`fast=FALSE`) or an implementation that relies on the `Rcpp` and `RcppArmadillo` packages (`fast=TRUE`).

The *wCorr Formulas* vignette describes the statistical properties of the correlation estimators in the package and has a more complete derivation of the likelihood functions.

## The ML switch

The correlation coefficients between two vectors of random variables that are jointly bivariate normal—call the vectors  $\mathbf{X}$  and  $\mathbf{Y}$ .

$$\begin{pmatrix} X \\ Y \end{pmatrix} \sim N \left[ \begin{pmatrix} \mu_x \\ \mu_y \end{pmatrix}, \Sigma \right]$$

where  $N(\mathbf{A}, \Sigma)$  is the bivariate normal distribution with mean  $\mathbf{A}$  and covariance  $\Sigma$ .

## Polyserial computation

the likelihood function for an individual observation of the polyserial is<sup>1</sup>

$$\Pr(\rho = r, \boldsymbol{\theta}; Z = z_i, M = m_i) = \phi(z_i) \left[ \Phi \left( \frac{\theta_{m_i+2} - r \cdot z_i}{\sqrt{1 - r^2}} \right) - \Phi \left( \frac{\theta_{m_i+1} - r \cdot z_i}{\sqrt{1 - r^2}} \right) \right]$$

where  $\rho$  is the correlation between  $\mathbf{X}$  and  $\mathbf{Y}$ ,  $\mathbf{Z}$  is the normalized version of  $\mathbf{X}$ , and  $\mathbf{M}$  is a discretized version of  $\mathbf{Y}$ , using  $\boldsymbol{\theta}$  as cut points as described in the *wCorr Formulas* vignette.

The log-likelihood is then

$$\ell(\rho, \boldsymbol{\theta}; z, m) = \sum_i w_i \ln [\Pr(\rho = r, \boldsymbol{\theta}; Z = z_i, M = m_i)]$$

The derivatives of  $\ell$  can be written down but are not readily computed and so when the `ML` argument is set to `FALSE` (the default) a one dimensional optimization of  $\rho$  is calculated using `stats::optimize`. When the `ML` argument is set to `TRUE` a multi-dimensional optimization is done for  $\rho$  and  $\boldsymbol{\theta}$  using `minqa::bobyqa`.

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<sup>1</sup>See the *wCorr Formulas* vignette for a more complete description and motivation for the polyserial correlations's likelihood function.

## Polychoric computation

For the polychoric the observed data is discreteized for both variables. Here the discretized version of  $\mathbf{X}$  is  $\mathbf{P}$  and the discretized version of  $\mathbf{Y}$  remains  $\mathbf{M}$ .<sup>2</sup> The likelihood function for the polychoric is

$$\Pr(\rho = r, \boldsymbol{\theta}, \boldsymbol{\theta}'; P = p_i, M = m_i) = \int_{\theta'_{p_i+1}}^{\theta'_{p_i+2}} dx \int_{\theta_{m_i+1}}^{\theta_{m_i+2}} dy f(x, y | \rho = r)$$

where  $f(x, y | r)$  is the normalized bivariate normal distribution with correlation  $\rho$ , and  $\boldsymbol{\theta}'$  are the cut points used to discretize  $\mathbf{X}$  into  $\mathbf{P}$ .

The log-likelihood is then

$$\ell(\rho, \boldsymbol{\theta}, \boldsymbol{\theta}'; \mathbf{p}, \mathbf{m}) = \sum_i w_i \ln [\Pr(\rho = r, \boldsymbol{\theta}, \boldsymbol{\theta}'; P = p_i, M = m_i)]$$

The derivatives of  $\ell$  can be written down but are not readily computed and so when the ML argument is set to **FALSE** (the default) a one dimensional optimization of  $\rho$  is calculated using `stats::optimize`. When the ML argument is set to **TRUE** a multi-dimensional optimization is done for  $\rho$ ,  $\boldsymbol{\theta}$ , and  $\boldsymbol{\theta}'$  using `minqa::bobyqa`.

## General setup for the unweighted case

A simulation is run several times. For each iteration, the following procedure is used:

- select the number of observations ( $n$ )
- select a true correlation coefficient  $\rho$
- generate  $\mathbf{X}$  and  $\mathbf{Y}$  to be bivariate normally distributed using a pseudo-Random Number Generator (RNG)
- using a pseudo-RNG, select the the number of bins for  $\mathbf{M}$  and  $\mathbf{P}$  ( $t$  and  $t'$ ) independantly from the set  $\{2, 3, 4, 5\}$
- select the bin boundaries for  $\mathbf{M}$  and  $\mathbf{P}$  ( $\boldsymbol{\theta}$  and  $\boldsymbol{\theta}'$ ) by sorting the results of  $(t - 1)$  and  $(t' - 1)$  draws, respectively, from a normal distribution using a pseudo-RNG
- confirm that at least 2 levels of each of  $\mathbf{M}$  and  $\mathbf{P}$  are occupied (if not, rerun to generating  $\mathbf{X}$  and  $\mathbf{Y}$ )
- calculate and record relevant statistics

When the exact method of selecting a parameter (such as  $n$ ) is not noted in the above description it is described as part of each simulation.

## ML switch

A simulation was done at each level of the cartesian product of  $\text{ML} \in \{\text{TRUE}, \text{FALSE}\}$ ,  $\rho \in (-0.99, -0.95, -0.90, -0.85, \dots, 0.95, 0.99)$ , and  $n \in \{10, 100, 1000\}$ . For precision, each iteration is run three times. The computation is run so that the same values of the variables are used for  $\text{ML}=\text{TRUE}$  as  $\text{ML}=\text{FALSE}$  and then the statistics are compared between the two sets of results. where  $MAD$  is the mean absolute difference and is given by

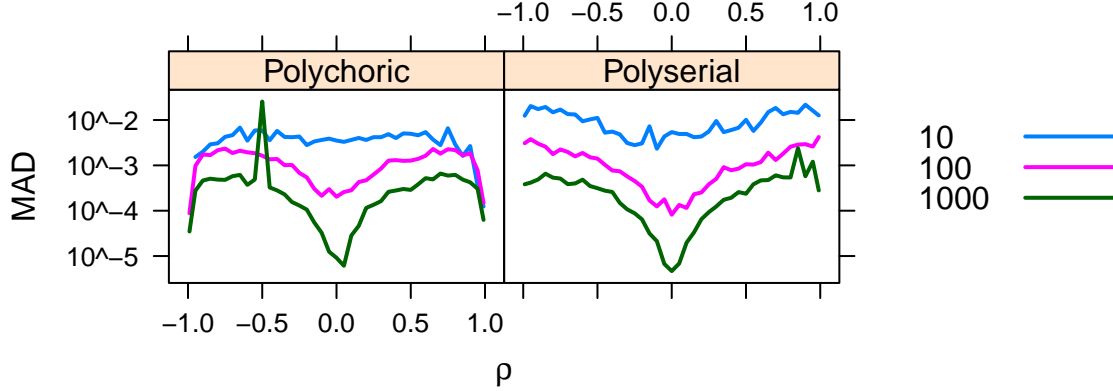
$$MAD = |r_{ML=TRUE} - r_{ML=FALSE}|$$

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<sup>2</sup>See the “wCorr Formulas” vignette for a more complete description and motivation for the polychoric correlations’s likelihood function.

where  $r_{ML=TRUE}$  is the estimated correlation when  $ML=TRUE$  and  $r_{ML=FALSE}$  is the estimated correlation when  $ML=FALSE$ .

This is a plot of the  $MAD$  as a function of the true correlation coefficient. It shows a decrease in  $MAD$  as  $n$  increases (change from line to line), a decrease when the correlations are in the neighborhood of zero that is more pronounced for larger  $n$  and a dip then the correlation is exactly 1 or -1.



This table shows the  $MAD$  by  $n$  and correlation type.

Correlation type	n	MAD
Polychoric	10	0.0037186
Polychoric	100	0.0012056
Polychoric	1000	0.0009111
Polyserial	10	0.0099031
Polyserial	100	0.0013888
Polyserial	1000	0.0003561

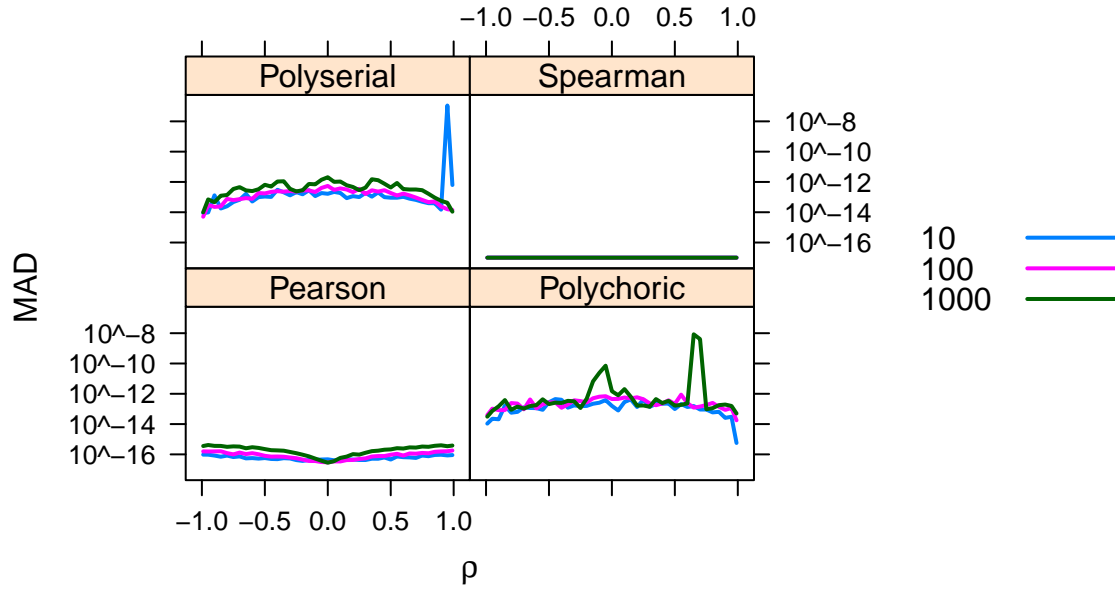
These results show that the side of the  $MAD$  decreases as  $n$  increases. When  $n = 10$ , the  $MAD$  is less than 0.02 for the polyserial and 0.002 for the polychoric.

## fast switch

This section looks at the agreement between the pure R implementation of the optimizations and the `Rcpp` and `RcppArmadillo` implementation. The code can compute with either option by setting `fast=FALSE` (pure R) or `fast=TRUE` (`Rcpp`).

A simulation was done at each level of the cartesian product of  $\text{fast} \in \{TRUE, FALSE\}$ ,  $\rho \in (-0.99, -0.95, -0.90, -0.85, \dots, 0.95, 0.99)$ , and  $n \in \{10, 100, 1000\}$ . Each iteration was run 100 times. The computation is run so that the same values of the variables are used for `fast=TRUE` as `fast=FALSE` and then the statistics are compared between the two sets of results.

This is the summary of all differences between the `fast=TRUE` and `fast=FALSE` runs for the polyserial. Note that differences smaller than  $10^{-16}$  are indistinguishable from 0 by the machine. However, a factor of  $10^{-17}$  was added to the results so that they could all be shown on a log scale. Thus the Spearman never shows differences that are different from zero.

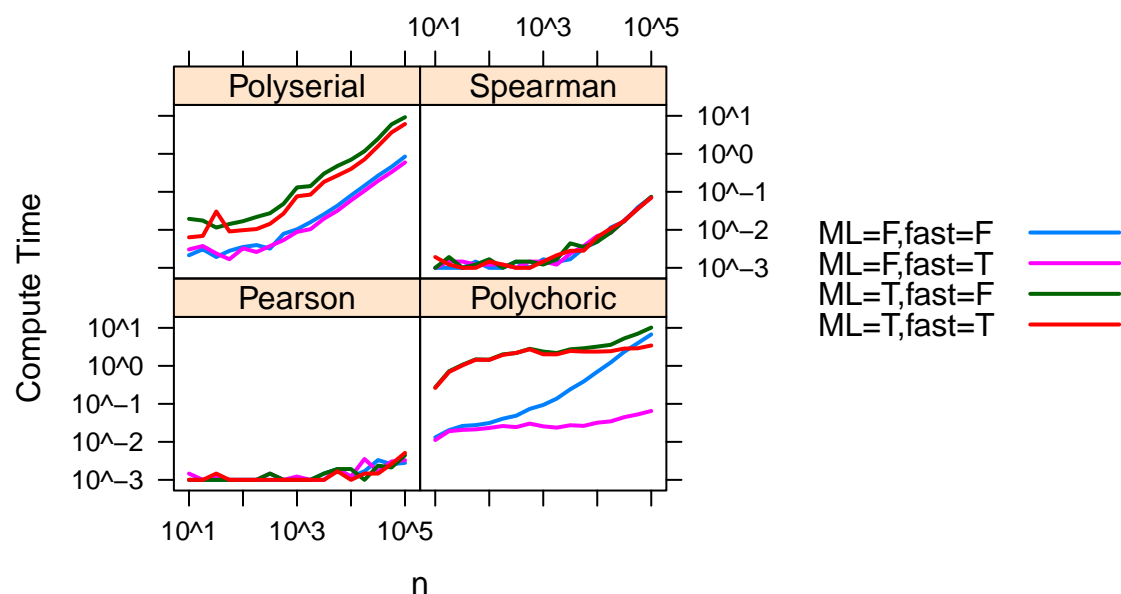


The above shows that differences as a result of the **fast** argument are never larger than  $10^{-8}$  for any type.

## Implications for speed

A simulation was done at each level of the cartesian product of  $ML \in \{\text{TRUE}, \text{FALSE}\}$ ,  $\text{fast} \in \{\text{TRUE}, \text{FALSE}\}$ ,  $\rho \in (-0.99, -0.95, -0.90, -0.85, \dots, 0.95, 0.99)$ , and  $n \in \{10^1, 10^{1.25}, 10^{1.5}, \dots, 10^7\}$ . For precision, each iteration is run 80 times when  $n < 10^5$  and 20 times when  $n \geq 10^5$ . The computation is run so that the same values of the variables are used all four levels of **ML** and **fast**. The variety of correlations is chosen so that the results represent an average of possible values of  $\rho$ .

The following plot shows the mean compute time versus  $n$ .



## Conclusion

Using tables presented in this vignette, users who wish to use the more accurate `ML=TRUE` argument can compare the difference in computation time and the difference in results.

the `fast` argument is provided primarily for comparison of the `Rcpp` and pure R code and shows agreement to within  $10^{-8}$ .